

Generalized Extensivity

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Abstract

In order to apply thermodynamics to systems in which entropy is not extensive, it has become customary to define generalized entropies. While this approach has been effective, it is not the only possible approach. We suggest that some systems, including nanosystems, can be investigated by instead generalizing the concept of extensivity. We begin by reexamining the role of linearity in the definition of complex physical systems. We show that there is a generalized form of extensivity that can be defined for a number of non-linear systems. We further show that a generalization of the principle of linear superposition is the basis for defining generalized extensivity. We introduce a definition for the degree of non-extensivity for systems. We show that generalized extensivity can be used as a means of understanding complex physical systems and we propose extending the idea extensivity beyond thermodynamics to other physical systems, including nanosystems.

Keywords: Tsallis Entropy, extensivity, generalized extensivity, nanothermodynamics

1. Introduction

A number of authors have proposed generalizations of entropy to address the problem of providing a universal measure of complexity or disorder, examples include Tsallis entropy, and Renyi entropy [1]. One of the properties of entropy that remains controversial is the issue of extensivity—the appearance of linear or additive behavior of the subcomponents of a system when taken as a whole. Extensivity is not a universal feature of entropy, though it is often treated as if it is [2, 3]. However, a variety of sources have demonstrated that entropic extensivity cannot be one of the fundamental axioms of thermodynamics, see [4] for further discussions.

To illustrate that extensivity is not a fundamental axiom of thermodynamics, we may consider a familiar example: entropy was defined phenomenologically by Clausius as an integral over a reversible path, but as Jaynes [5] observed the Clausius definition says nothing about extensivity, since the size of the system does not vary over the integration path. Furthermore, Hill, in pioneering work in the 1960s noted that extensivity does not apply to all entropic systems, particularly those which exist at small scales [6–8]. Thus, extensivity is a notion independent of entropy. The subject of this paper is how to generalize

extensivity so it applies to more general complex systems. There is an advantage in attempting to generalize what can be thought of as a purely mathematical concept. Extensivity can be generalized in a straightforward manner without bringing along the physical ideas associated with entropy; in this way we can avoid the confusion that often arises from mixing the physical and mathematical aspects of entropy.

In complex, compound systems, the meaning of extensivity needs to be explored in order to gain insight into the meaning of complexity. Instead of proposing yet another generalization of entropy, we will show that the notion of extensivity can be generalized. Generalized extensivity allows us to replace the classical notion of extensivity by considering a more general notion of superposition. By choosing to broaden the notion of what constitutes an extensive system rather than changing the notion of what classical entropy means, we choose to economize the physical interpretation of entropy; this serves an economy of purpose consistent with Occam's razor.

We take a contrarian viewpoint to the proposed generalization of entropy by Tsallis [9] as well as many subsequent ideas that are summarized in [10]. This approach allows us to suggest an approach to addressing the following the point made by Boon and Tsallis [11]:

Asking whether the entropy of a system is or is not extensive *without indicating the composition law of its elements*, is like asking whether

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some body is or is not in movement *without indicating the referential with regard to which we are observing the velocity.*

The formalism of *generalized superposition* can be used to ask what type of functions allow a nonlinear combination to give the appearance of superposition.

We suggest several different forms of generalized extensivity can be defined, including one associated with power laws which is connected to Tsallis entropy. As part of this exploration, we cast Tsallis entropy in a manner that is consistent within the framework of generalized extensivity. Thus, instead of being concerned whether Tsallis entropy has the appearance of extensivity or when it is inherently non-extensive, we propose that it can be viewed as having the property of extensivity in the same context that a law of generalized superposition can be found, e.g. when it can be related to power laws. We also discuss the role generalized superposition plays in the understanding of power laws.

2. The Principle of Superposition and Generalized Extensivity

The notion of extensivity can be developed mathematically by relating it to the theory of linear systems. For a linear system with inputs $x_i(n)$, scalars c_i and a system transform $T()$ there is always a rule for combining inputs to give outputs. This system will be linear, provided the system obeys the principle of superposition (where $+$ denotes ordinary addition)

$$T[x_1(n) + x_2(n)] = T[x_1(n)] + T[x_2(n)] \quad (1)$$

and scalar multiplication \cdot

$$T[c \cdot x(n)] = c T[x(n)] \quad (2)$$

There are many physical quantities where combinations behave like linear systems and obey the principle of superposition. Mass and energy are examples of quantities that exhibit this property, when individual components of mass and energy are combined, the result is the combination of the individual masses and energies. Thus both mass and energy are extensive variables. On the other hand, temperature is not extensive because it is not additive over sub-systems.

The most familiar example of a combination of components that is not extensive is multiplication. For a system with a law of combination defined by multiplication:

$$x(n) = [x_1(n)] \cdot [x_2(n)] \quad (3)$$

with the introduction of a separator function for multiplication, the logarithm,

$$\begin{aligned} \log x(n) &= \log ([x_1(n)] \cdot [x_2(n)]) \\ &= \log [x_1(n)] + \log [x_2(n)]. \end{aligned} \quad (4)$$

we have the appearance of superposition. For example, the Boltzmann definition of entropy is $S = k \ln \Omega$, so under the circumstances that the microstates are multiplicative $\Omega = \Omega_1 \Omega_2$, then the entropy of the combined states is $S = S_1 + S_2$; so the Boltzmann entropy obeys the principle of generalized extensivity. We then introduce the definition

$$S = \log[x(n)], \quad (5)$$

so that Eq. (4) becomes

$$S = S_1 + S_2. \quad (6)$$

This is an example of a non-linear combination of components that can be re-interpreted as obeying superposition principle. This suggests that we can look for an underlying generalized superposition principle, that is extensivity, in many complex systems. Such a principle exists in signal processing, in the analysis of homomorphic systems, that has wider applications in complex systems as we now discuss.

2.1. Generalized Extensivity

In order to generalize the idea of superposition in linear systems to non-linear systems, Oppenheim [12] proposed a modification of Eq. (1) and Eq. (2). The summation sign in Eq. (1) must be replaced with two different symbols: a rule for combining inputs designated by \otimes , and a rule for combining outputs designated by \oplus . We then write the generalized superposition principle for such a system with a system transform $H()$ as

$$H[x_1(n) \otimes x_2(n)] = H[x_1(n)] \oplus H[x_2(n)] \quad (7)$$

which is the generalization of Eq. (1) for nonlinear systems. A similar replacement is required for scalar multiplication by a constant c , so the generalization of Eq. (2) is

$$H[c \otimes x(n)] = c \circ H[x(n)] \quad (8)$$

where \otimes replaces the input scalar multiplication and \circ replaces the output scalar multiplication. The notation we have adopted is an adaptation of the notation used in the signal processing literature [13].

Systems with inputs and outputs that satisfy both (7) and (8) are called *homomorphic systems* since they can be represented as algebraically linear (homomorphic) mappings between the input and output signal spaces. Oppenheim and Schaffer have written a brief history of signal processing background for solving certain non-linear signal processing problems which are the origin of their classification scheme [14]. They summarized this informally, by stating that all homomorphic systems can be thought of in the following manner:

... all homomorphic systems have canonical representation consisting of a cascade of three systems. The first system is an invertible nonlinear characteristic operator (system)

that maps a nonadditive combination operation such as a convolution into ordinary addition. The second system is a linear system obeying additive superposition, and the third system is the inverse of the first nonlinear system.

The logarithmic function is a separator function for multiplication. That is why there is confusion about entropy being extensive, for many systems the total entropy is achieved by the multiplication of subsystems, but this is not always true. Hill [6] includes examples where multiplication over subsystems does not yield the true entropy of the composite system.

Most non-linear functions $N(x, y)$ do not separate with a superposition principle, for example a separator function S does not exist such that

$$S[N(x, y)] = A(x) + B(y). \quad (9)$$

The mathematical details for determining if the rule for combining systems can be deconstructed so that a valid separator function S exists are discussed by Tretiak and Eisenstein [15].

An informal argument is sufficient for our purposes to capture the flavor of the conditions for S to be a separator function. By taking the partial derivative ($f_{,x} \triangleq \frac{\partial f}{\partial x}$) of Eq. (9) with respect to each of the individual arguments, we have

$$S'[N(x, y)]N_{,x}(x, y) = A_{,x}(x), \quad (10)$$

and

$$S'[N(x, y)]N_{,y}(x, y) = B_{,y}(y); \quad (11)$$

combining we find

$$\frac{N_{,x}(x, y)}{N_{,y}(x, y)} = \frac{A_{,x}(x)}{B_{,y}(y)}. \quad (12)$$

Then, by defining

$$H(x, y) = \ln \left(\frac{N_{,x}(x, y)}{N_{,y}(x, y)} \right) = \ln A_{,x}(x) - \ln B_{,y}(y), \quad (13)$$

we see that

$$H_{,x}(x, y) = \frac{A_{,xx}(x)}{A_{,x}(x)}, \quad (14)$$

and

$$H_{,y}(x, y) = -\frac{B_{,yy}(y)}{B_{,y}(y)}; \quad (15)$$

thus the first partials of $H(x, y)$ are functions of a single variable and separation has been achieved. This provides the means of finding a separator function for $N(x, y)$. In thermodynamic language, the existence of a separator function means that there is a Maxwell relation between the variables A and B .

Generalized superposition provides an interpretation of the extensivity property of entropy when it exists. In fact,

generalized superposition can be used as a guiding principle to look for extensive variables in a generalized setting [16, 17] of determining the thermodynamics of complex systems. More general types of entropy-like variables can be defined using this form of generalized superposition. Since the rule for combining subsystems into the whole is nonlinear, the principle of generalized superposition allows us to look for a rule that gives the appearance of linearity, and hence extensivity. Linearity on a macroscopic scale gives us a generalized thermodynamics of complex systems. The realization that the counting functions that enumerate the states have an underlying separator function that obey this generalized form of superposition allows us to generalize the concept of extensivity. Thus, we define a system as obeying a principle of *generalized extensivity* if it obeys Eqs. (7) and (9) rather than Eqs. (1) and (2).

2.2. Other Forms of Extensivity

A second possibility that allows us to consider another type of extensivity is illustrated by considering a relaxation of the linearity requirement. An enumeration function need not be strictly linear either. An example of this is illustrated by attempting to linearize a counting function such as the factorial $n!$. While $\ln(n!)$ is not linear, it is approximately linear for a physical system that has a large number of components; thus for all practical purposes

$$\ln((n+m)!) \approx n \ln(n) + m \ln(m) \approx \ln(n!) + \ln(m!); \quad (16)$$

so $n!$ has been linearized with respect to the logarithm. We have omitted a factor $O(\frac{1}{n})$ in Eq. 16, this term is ignorable in systems that consist of a significant number of interacting units. The only time this factor plays a role is when trying to determine the transition point between collective and individual behavior, such as in the question of how many atoms are required before a system acts like a liquid or solid, or at the nanoscale where collective behavior starts to break down. (We will discuss this question further in a subsequent paper – it is largely outside of the purview of this paper.) The difference between approximately linear and linear is a point that is not emphasized as examining the factorial function illustrates. There are a number of different functions that are linear in the Stirling approximation. This notion of extensivity is captured by what we term *Ulam extensivity* that is related to the mathematical properties of functions that are termed approximately linear [18–20]. Consider

$$f(x+y) - f(x) - f(y) \approx C + O(g(x)), \quad (17)$$

where $g(x)$ tends to 0 as x becomes large, which is the reason the logarithm of a factorial gives the appearance of linearity for large n . Vogt [21] has discussed form isometry which could be considered as a means to generalize Ulam extensivity.

2.3. Power Laws, Homogeneity, and Extensivity

Generalized extensivity connects power laws and homogeneity together. To illustrate the concept of generalized extensivity we consider an example of a system that has a power-law like combination rule for counting combinations of states which is defined by

$$x(n) = [x_1(n)]^\alpha \cdot [x_2(n)]^\beta \quad (18)$$

where α and β are constants. Notice that with the introduction of a separator function for multiplication, the logarithm, we have

$$\begin{aligned} \log(x(n)) &= \log([x_1(n)]^\alpha \cdot [x_2(n)]^\beta) \\ &= \alpha(\log[x_1(n)]) + \beta(\log[x_2(n)]). \end{aligned} \quad (19)$$

Thus recovering a familiar superposition principle. If we then chose $\alpha = \beta$, we have

$$\log(x(n)) = \alpha(\log[x_1(n)] + \log[x_2(n)]).$$

This equation reminds us of the basic definition of extensivity through the theory of homogeneous functions. We will now review the basic ideas through which we can analyze power laws using generalized extensivity.

The functional equations appropriate to the study of homogenous functions were developed by Euler [22, 23]. Davis [24], Stanley [25], and Widder [26] provide modern introductions of varying degrees of sophistication to functional equations. In general, a function $f(x)$ is a homogenous function, if for all values of the parameter λ ,

$$f(\lambda x) = g(\lambda)f(x) \quad (20)$$

Stanley [25] has shown that g is not arbitrary function, instead it is the parameter raised to a power of n . Thus a homogenous function $f(x)$ is one that satisfies

$$f(x\lambda) = \lambda^n f(x) \quad (21)$$

This definition can be extended to any finite number of variables. The degree, n , is restricted to integer values only. It is possible for multidimensional functions to be homogenous of different degrees for different variables. This is common occurrence in thermodynamics. For a function in the variables x , y , and z ; the function satisfies

$$f(\lambda x, \lambda y, z) = \lambda^n f(x, y, z), \quad (22)$$

we say this function is homogenous of degree n in the variables x and y which it is not homogenous in the variable z . A definition introduced by Stanley [25] of a generalized homogeneous function, is that it is a function that satisfies the equation

$$f(\lambda^a x, \lambda^b y) = \lambda f(x, y). \quad (23)$$

It is this formulation of homogenous functions that is widely used in the analysis of critical point phenomena and phase transitions using the static scaling hypothesis. Functions

that are homogenous obey the principle of generalized superposition since $f(x\lambda) = \lambda^n f(x)$ and $f(y\lambda) = \lambda^n f(y)$ so in general $\lambda^n f(x) + \lambda^n f(y) \neq f(\lambda x + \lambda y)$, however for $n = 1$, we have

$$\begin{aligned} \lambda f(x) + \lambda f(y) &= f(x\lambda) + f(y\lambda) \\ &= f(\lambda x + \lambda y) = f(x + y), \end{aligned} \quad (24)$$

so homogeneity and extensivity are the same for some types of functions. This form of extensivity is what we term *homogenous extensivity*.

2.4. Symbolic Extensivity

The concept of *symbolic extensivity* arises naturally from dimensional analysis. Three approaches can be taken based on the common aegis of dimensional analysis codified by Bridgman [27]. You can take all the physical units that are required for a complete system specification of a physical group of functions such as length L , time T , mass M , etc.; so the dimensional symbols action under the operations of arithmetic constitute a mathematical group. For example, consider the symbol for length L . Combinations of L form a group \mathcal{G}_L : there is an identity, $L^0 = 1$; there is an inverse, $1/L$ or L^{-1} ; and L raised to any rational power p is a member of \mathcal{G}_L which has an inverse L^{-p} . The group operation is multiplication, with the usual rules for handling exponents ($L^n \times L^m = L^{n+m}$). For example in classical mechanics, any physical quantity can be expressed dimensionally in terms of base units which have dimensions M , L , and T .

From this group specification, by noting that by replacing a variable x in $f(x)$ by $(x + \delta_x)$, it is natural to define $f(x)$ to be *translationally extensive* if

$$f(x + \delta_x) = f(x) + f(\delta_x). \quad (25)$$

The *degree of non-extensivity* $\Xi(x, \delta_x)$ of a function $f(x)$ is then

$$\frac{f(x + \delta_x) - f(x) - f(\delta_x)}{f(x)} = \Xi(x, \delta_x); \quad (26)$$

so $\Xi(x, \delta_x) = 0$ for an extensive function. For a function that is Ulam extensive,

$$\Xi(x, \delta_x) = \frac{C}{g(x)} \quad (27)$$

which is effectively zero for almost all $g(x)$, especially those that scale with the number of objects. As an example, the area of square of side x is x^2 , so $f(x) = x^2$, then $\Xi(x, \delta_x) = \frac{\delta_x}{x}$, so for $\delta_x \ll x$, $\Xi(x, \delta_x) \simeq 0$ and area of square is approximately extensive; however, when x becomes comparable in size to δx the area is non-extensive. This behavior is potentially observable at the transition from macrosystems to nanosystems. To extend the definition to multiple dimensions, we define the degree of non-

extensivity as

$$\frac{f(x_1 + \delta_{x_1}, x_2 + \delta_{x_2}, \dots, x_n + \delta_{x_n}) - f(\vec{x}) - f(\vec{\delta_{\vec{x}}})}{f(\vec{x})} = \Xi(\vec{x}, \vec{\delta_{\vec{x}}}). \quad (28)$$

A multidimensional function is translationally extensive if $\Xi(\vec{x}, \vec{\delta_{\vec{x}}}) = 0$. The volume of a cylinder is $\pi l r^2$, so the degree of non-extensivity is

$$\begin{aligned} \Xi(r, \delta_r, l, \delta_l) &= \frac{f(r + \delta_r, l + \delta_l) - f(r, l) - f(\delta_r, \delta_l)}{f(r, l)} \\ &= 2\frac{\delta_r}{r} + \frac{\delta_r^2}{r^2} + \frac{\delta_l}{l} + 2\frac{\delta_r \delta_l}{lr} \end{aligned}$$

It is only when the fractional terms scale with the dimensional ratios, $\frac{\delta_r}{r}$ and $\frac{\delta_l}{l}$, that the degree of non-extensivity is not effectively zero. For most volumes for which we have an analytical formula, they can be translationally extensive until the dimensional ratios, $\frac{\delta_r}{r}$ and $\frac{\delta_l}{l}$, are of similar size, then extensivity breaks down in a non-linear fashion.

The dimensional specification group, \mathcal{G}_S , is constituted from the individual units of the dimensional quantities that constitute the units of the overall complex system which are labeled U_1, U_2, \dots, U_n in the system specification which are specified by the groups $\mathcal{G}_{U_1}, \mathcal{G}_{U_2}, \dots, \mathcal{G}_{U_n}$. The complex system group is obtained by taking the direct product, \otimes , of these groups :

$$\mathcal{G}_S = \mathcal{G}_{U_1} \otimes \mathcal{G}_{U_2} \otimes \dots \otimes \mathcal{G}_{U_n}. \quad (29)$$

It is possible to use the complex system group to formulate a dimensionless specification for each complex system units provided they are specified by scaling factors. Thus, for a complex physical system specified by variables x_1, x_2, \dots, x_n , can be represented as $P(x_1, x_2, \dots, x_n)$. The way to remove the dimensions from a physical variable is to replace $x_1 \rightarrow \delta_{x_1} x_1$ where δ_{x_1} has units proportional $\frac{1}{x_1}$, A function that satisfies

$$f(\epsilon_{x_1} x_1) = g(\epsilon_{x_1}) f(x_1)$$

which is scaling or homogenous extensivity. Necessarily, since

$$\lim_{\epsilon_{x_1} \rightarrow 1} f(\epsilon_{x_1} x_1) = f(x_1) \quad (30)$$

which means $\lim_{\epsilon_{x_1} \rightarrow 1} g(\epsilon_{x_1}) = 1$. So by an argument similar to the one used by Stanley in the previous section $g \sim x^n$. So this type of extensivity reduces essentially to earlier work.

3. Discussion and Conclusions

The notion of extensivity extends beyond physics to the entire subject of complex systems [28]. While the survey by Tsallis and Gell-Mann discusses many non-physics

applications of Tsallis entropy [29], we would argue that the same applies to generalized extensivity for much the same reasons. Furthermore, extensivity and its generalization applies to a new area of physics that is just starting to be explored: nanothermodynamics, a name that has been proposed by Hill [30, 31]. Nanothermodynamics requires that chemical potential as well as variables that are extensive require a reformulation by scaling them, not relative to one scaling component N , but rather rescaling the multiple components relative to scales of different sizes N_i . The appearance of collective behavior, e.g. nanothermodynamics, emerges only if the collective components act together in a unified manner, a type of generalized extensivity [32].

In conclusion, we have proposed a means of extending the concept of extensivity to a wider variety of physical systems as well as to the wider subject area of complex systems. As a result of this, we have suggested that the Tsallis entropy could be interpreted as a form of generalized superposition for some power laws.

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5. References

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